Supplementary Materials for

AI-assisted design of 3D NPR lattice materials with programmable mechanical properties via irregular unit cells

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This PDF file includes:

Figs. S1 to S3
Tables S1 to S2

Other Supplementary Materials for this manuscript include the following:

Movies S1 to S5

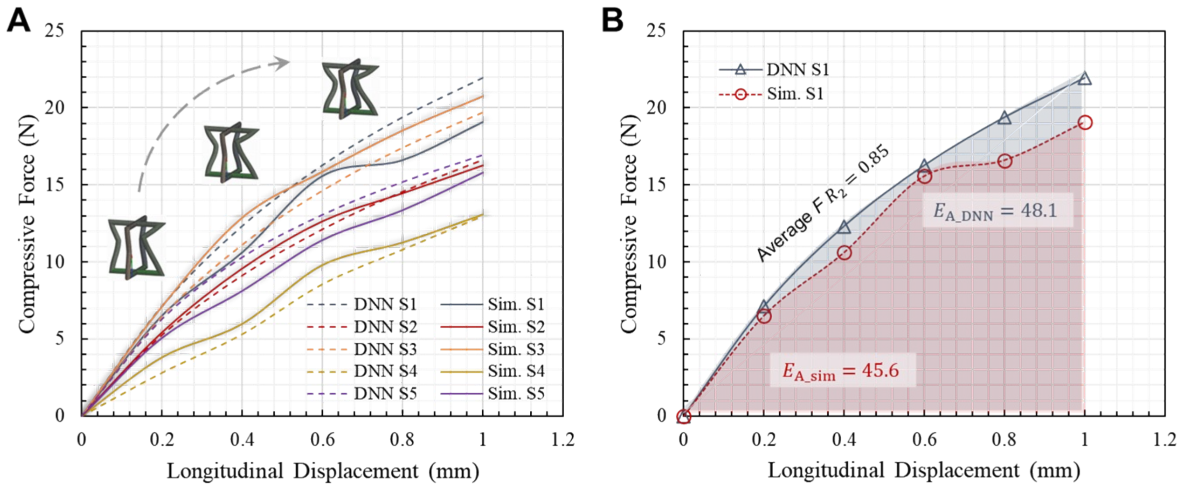

Fig. S1. Validation of DNN model for energy absorption prediction. (**A**) Force–displacement curves from numerical simulation and DNN predictions for five randomly selected unit cells. Overall trends align closely, though minor discrepancies occur at certain loading stages, contributing to the relatively lower R^2 value in force prediction. (**B**) Comparison of energy absorption values between simulation and DNN results for sample S1. Despite an average R^2 of 0.85 for force prediction, the DNN-derived energy absorption remains highly consistent with simulated results with less than 6% error.

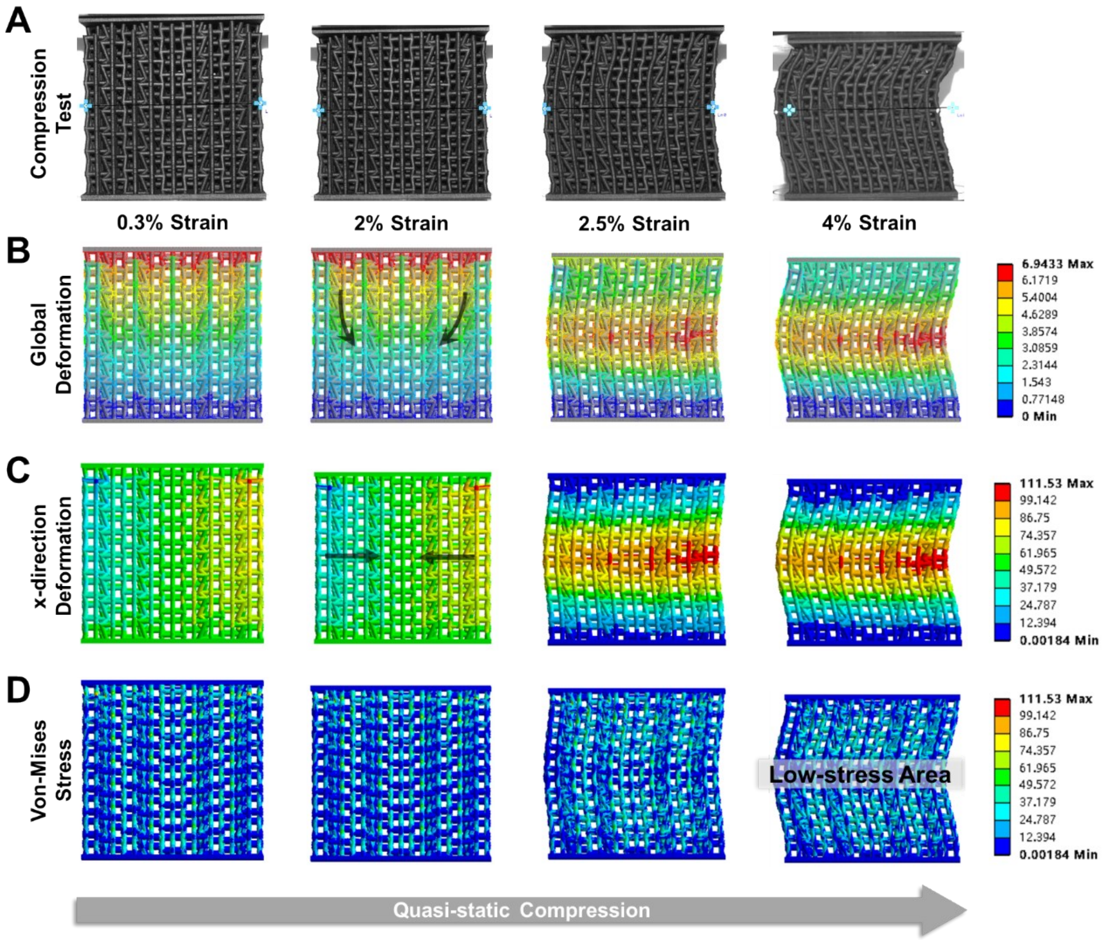

Fig. S2. Quasi-static compressive behavior of the macroscale irregular NPR lattice material. (**A**) Global deformation of the sample at 0.3%, 2%, 2.5%, and 4% longitudinal strain. Buckling initiates after 2.5% strain. (**B**) Simulated global deformation and (**C**) x-direction deformation, showing increasing strain localization toward the center prior to buckling. (**D**) Simulated Von-Mises stress distribution, revealing a low-stress region in the central buckling zone.

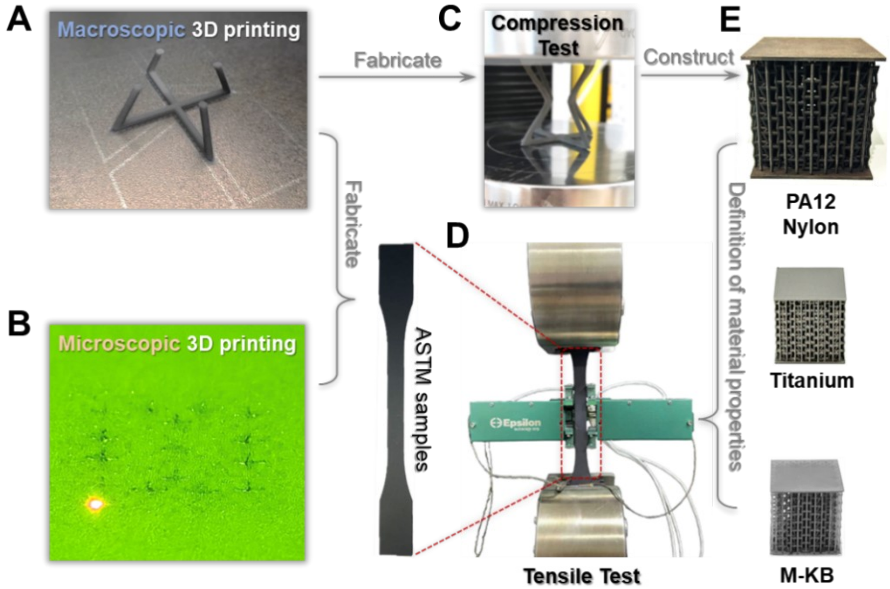

Fig. S3. Material property calibration and testing samples fabrication. (**A**) Fabrication of the base unit cell and ASTM-standard tensile specimens. (**B**) Quasi-static compressive testing of the base cell structure for validation against numerical simulations. (**C**) Manufacturing process for microscale lattice samples. (**D**) ASTM specimens produced via macro- and micro-scale 3D printing. Tensile tests on these specimens determine material properties for lattice simulations. (**E**) Macro- and micro-scale lattice samples used in compressive performance tests.

Table S1. Hyperparameters of the deep neural network (DNN) and genetic algorithm (GA) models. The DNN model comprises six hidden (dense) layers with a gradient-decent numbers of neurons. In these hidden layers, leaky_relu activation function is employed with a 0.3 dropout rate for each hidden layer. The last layer (output layer) contains a single neuron, while it output $\mu_{x,}\,\mu_x$ and E_A by altering the output data. The hyperparameters of the GA are tuned to be the given values by achieve good convergency of the loss function.

Machine learning models				
Deep Neuron Networks			Genetic Algorithm	
Dense layer 01	128 neurons	Activation function: *'leaky_relu'* Dropout rate: 0.3	Population Size	1000
Dense layer 02	96 neurons		Max Generation	500
Dense layer 03	72 neurons		Crossover Rate	0.9
Dense layer 04	48 neurons		Mutation Rate	0.2
Dense layer 05	24 neurons		Objective	*Maximum*
Output Layer 05	1 neuron	Activation function: *'linear'*		
Epochs	2000	/		
Batch Size	50	/		

Table S2. Geometric parameter definitions and relational descriptions for the irregular unit cell and its auxiliary cells. Column headers denote the base cell and auxiliary cells generated via rotational and mirror symmetry operations. Row labels (e.g., Neg./Pos. x/y-) indicate design points located along negative/positive x- or y-directions. The latter part -x, -y or -z of the subscript specify their spatial ordinates. Inter-cell relationships incorporate *Hz*, the fixed cell height determined by the overall dimensions.

	Basic Cell	**Cell Sx**	**Cell Sy**	**Cell Sxy**
Neg. x-x	P_{Nx_1}	$-P_{Px\_1}$	P_{Nx_1}	$-P_{Px\_1}$
Neg. x-y	P_{Nx_2}	$-P_{Px\_2}$	P_{Nx_2}	$-P_{Px\_2}$
Neg. x-z	P_{Nx_3}	$H_z - P_{Px\_3}$	P_{Nx_3}	$H_z - P_{Px\_3}$
Neg. y-x	P_{Ny_1}	P_{Ny_1}	$-P_{Py\_1}$	$-P_{Py\_1}$
Neg. y-y	P_{Ny_2}	P_{Ny_2}	$-P_{Py\_2}$	$-P_{Py\_2}$
Neg. y-z	P_{Ny_3}	P_{Ny_3}	$H_z - P_{Py\_3}$	$H_z - P_{Py\_3}$
Pos. x-x	P_{Px_1}	$-P_{Nx\_1}$	P_{Px_1}	$-P_{Nx\_1}$
Pos. x-y	P_{Px_2}	$-P_{Nx\_2}$	P_{Px_2}	$-P_{Nx\_2}$
Pos. x-z	P_{Px_3}	$H_z - P_{Nx\_3}$	P_{Px_3}	$H_z - P_{Nx\_3}$
Pos. y-x	P_{Py_1}	P_{Py_1}	$-P_{Ny\_1}$	$-P_{Ny\_1}$
Pos. y-y	P_{Py_2}	P_{Py_2}	$-P_{Ny\_2}$	$-P_{Ny\_2}$
Pos. y-z	P_{Py_3}	P_{Py_3}	$H_z - P_{Ny\_3}$	$H_z - P_{Ny\_3}$

Movie S1 to S5

Movie S1. In-situ compression of micro-sample with M-KB

Movie S2. Micro-DIC results of micro-sample with M-KB

Movie S3. In-situ compression of micro-sample with Titanium

Movie S4. Micro-DIC results of micro-sample with Titanium

Movie S5. Compression test of macro-sample with PA12 Nylon